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Supporting Information for

Meso-Substituted Bisanthenes as Soluble and Stable Near-infrared Dyes

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1. Photo-stability test of 4, 5 and 6 upon irradiation with UV lamp

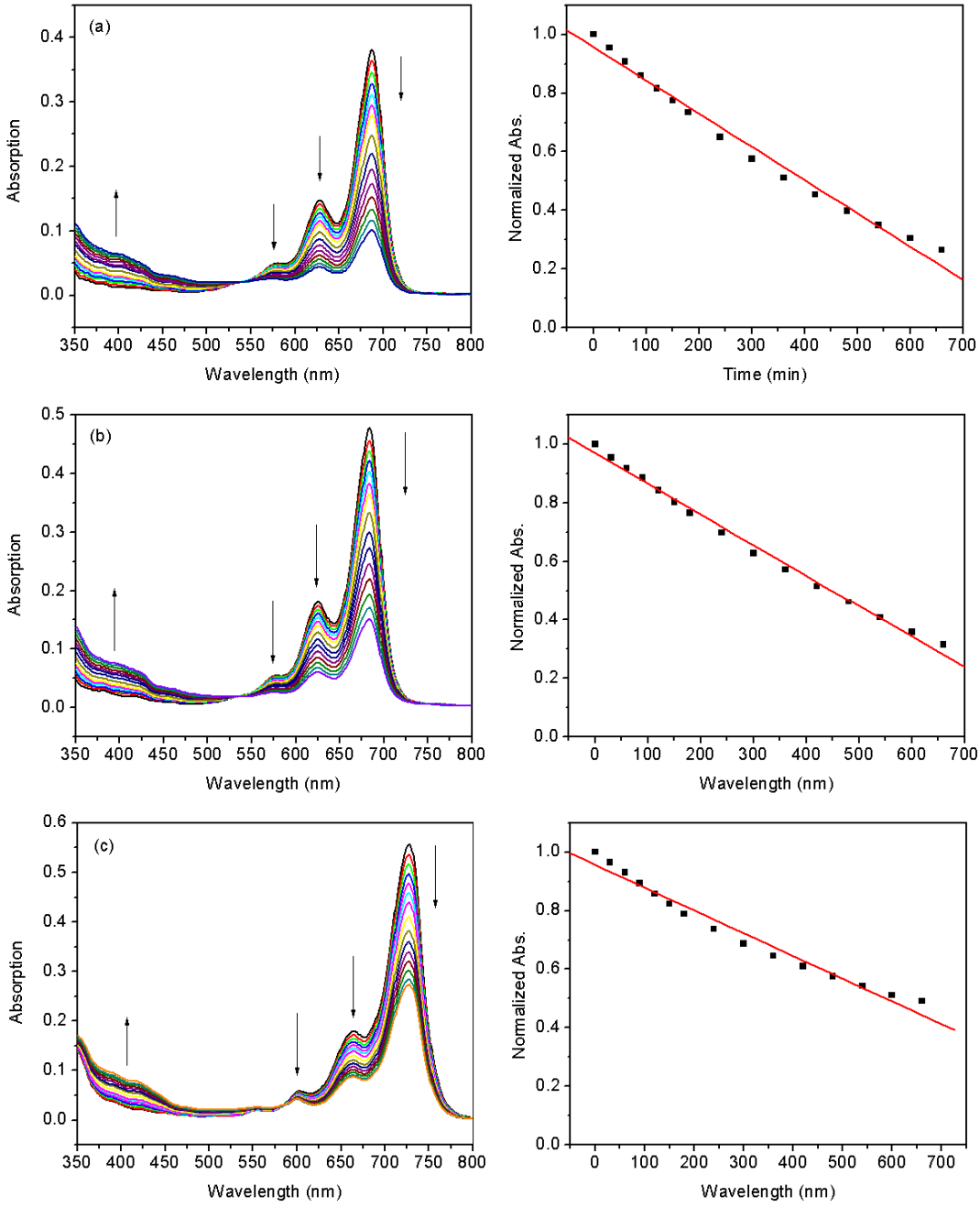


Figure S1. Photo-stability test of **4** (a), **5** (b) and **6** (c) in toluene upon irradiation of 4 W UV-light. Left: UV-vis-NIR absorption spectra of **4**, **5** and **6** in toluene recorded during the irradiation. Right: the change of the optical density at the absorption maximum with the irradiation time.

2. Thermogravimetric analysis (TGA) curves of 4, 5, and 6.

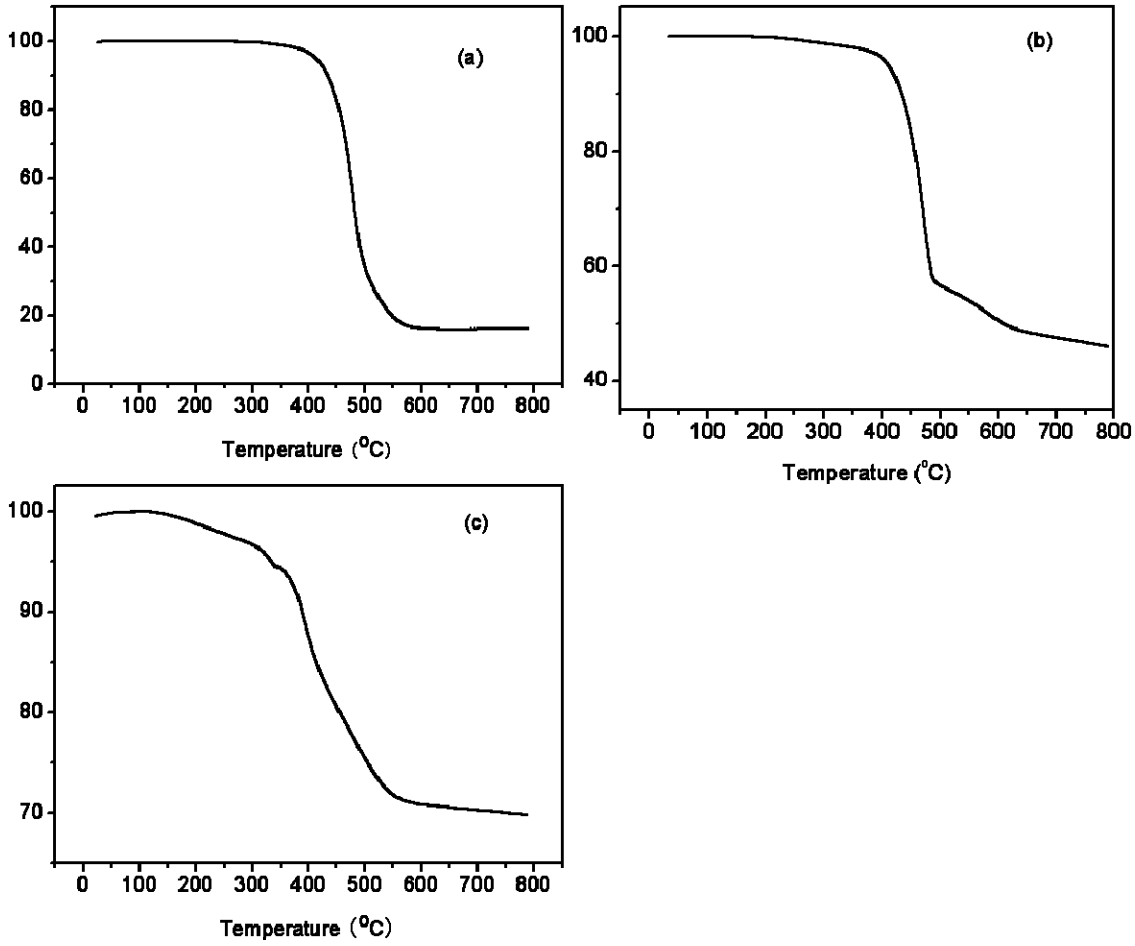


Figure S2. TGA curves of **4** (a), **5** (b) and **6** (c) (heating rate = 10 °C/min).

3. HR-EI mass spectra of 4, 5, 6, 8a and 8b

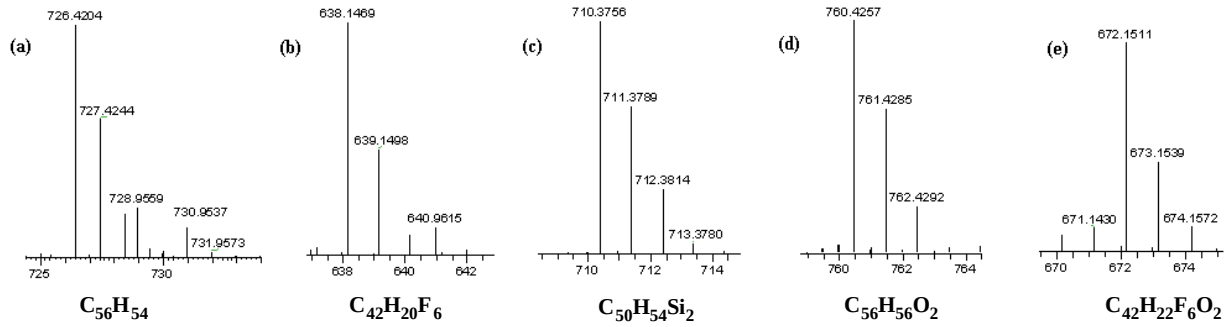


Figure S3. HR-EI mass spectra of **4** (a)**, 5** (b), **6** (c), **8a** (d) and **8b** (e).

4. Chemical oxidation titration of 4, 5 and 6

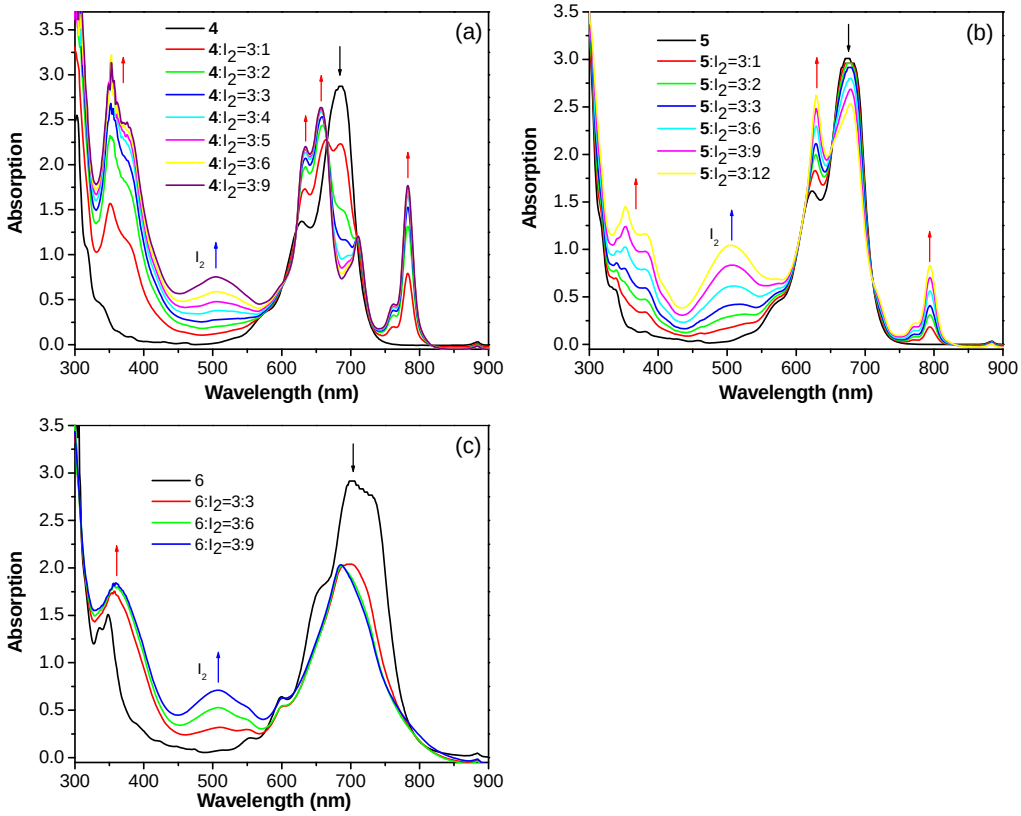


Figure S4. UV-vis-NIR absorption spectra of **4** (a), **5** (b) and **6** (c) during the titration by I_2 in dry DCM

5. TD-DFT calculation details

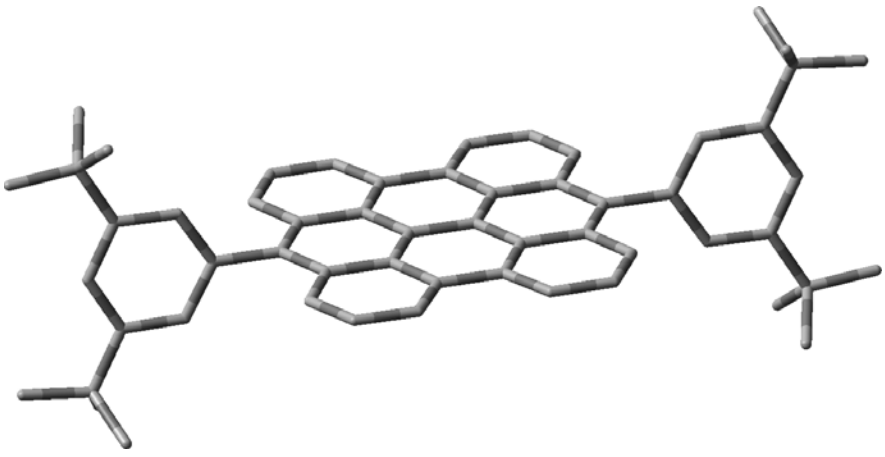
Time-dependent DFT (TD-DFT) calculations were performed using the *Gaussian03* (G03) program[1] at the B3LYP/6-31G** level of theory.[2-6] The geometries of **4**, **5**, and **6** were fully optimized in gas phase using the default convergence criteria without any constraints and confirmed by frequency calculations.

Table S1. Summary of calculated optical transitions

	calcd. (nm)	exp. (nm)	*f*	composition
4	716.3	687	0.4173	HOMO->LUMO (68%)
5	714.4	683	0.3856	HOMO->LUMO (67%)
6	785.6	727	0.5781	HOMO->LUMO (64%)

Cartesian Coordinates for DFT Calculated Optimized Structures and Selected Molecular Orbitals (contour value: 0.03):

Compound 4:



Sum of electronic and zero-point Energies= -2165.763466 (Hartree/Particle)

Sum of electronic and thermal Enthalpies (298.15 K) = -2165.712699

Sum of electronic and thermal Free Energies (298.15 K) = -2165.849471

	X	Y	Z
C	-3.49527825	2.00576526	-3.05491396
C	-2.56065108	1.70678629	-2.07135369
C	-2.32416204	2.66632650	-1.02733841
C	-3.05776339	3.90922209	-1.02877404
C	-4.00742446	4.14725381	-2.06597188
C	-4.21419485	3.21573111	-3.05126922
C	-1.38249981	2.40115402	-0.00126444
C	-2.83740069	4.86325184	-0.01106491
C	-1.89922639	4.60170804	1.01179154
C	-1.16458467	3.35952994	1.02031661
C	-0.21266752	3.11041223	2.06849200
C	-0.02677919	4.07936172	3.04663939
C	-0.73985758	5.29269125	3.03340472
C	-1.65280952	5.55467008	2.04388158
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C	-0.85997313	0.19083700	-1.01834411
C	0.29936733	0.88389167	1.02949442
C	-1.81182990	0.43997968	-2.06657049
C	-0.12520756	-1.05126764	-1.00991033
C	1.03285698	-0.35906606	1.03101458
C	0.53571425	1.84334982	2.07361145
C	-1.99720845	-0.52867809	-3.04509922

C	-0.37123705	-2.00401830	-2.04229923
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C	1.98210030	-0.59734432	2.06852144
C	1.46975256	1.54402034	3.05763220
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H	0.17407518	-2.93975719	-2.03167664
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H	-7.72618411	9.22294597	0.49164495
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H	-5.65046841	8.14652034	3.46426117
H	-7.26368944	7.47027690	3.75265591
H	-5.92884813	6.40992979	3.28291228
C	-3.29393072	9.15912270	-3.17284309
H	-2.91652007	9.96858577	-3.80791656
H	-2.64758277	8.28960272	-3.32271546
H	-4.29721972	8.89363569	-3.52206240
C	-1.89255332	9.98078606	-1.24107812
H	-1.88487855	10.30961262	-0.19667337
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H	-1.50059159	10.79798797	-1.85713861
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H	-5.22691347	10.68022662	-1.92966248
H	-4.24480138	11.25625854	-0.56890785
H	-3.78585931	11.65622007	-2.22630293

C	4.34889000	-3.84528463	-3.11729207
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H	5.24207638	-3.91823317	-3.74810760
H	3.62831287	-4.59419310	-3.46216672
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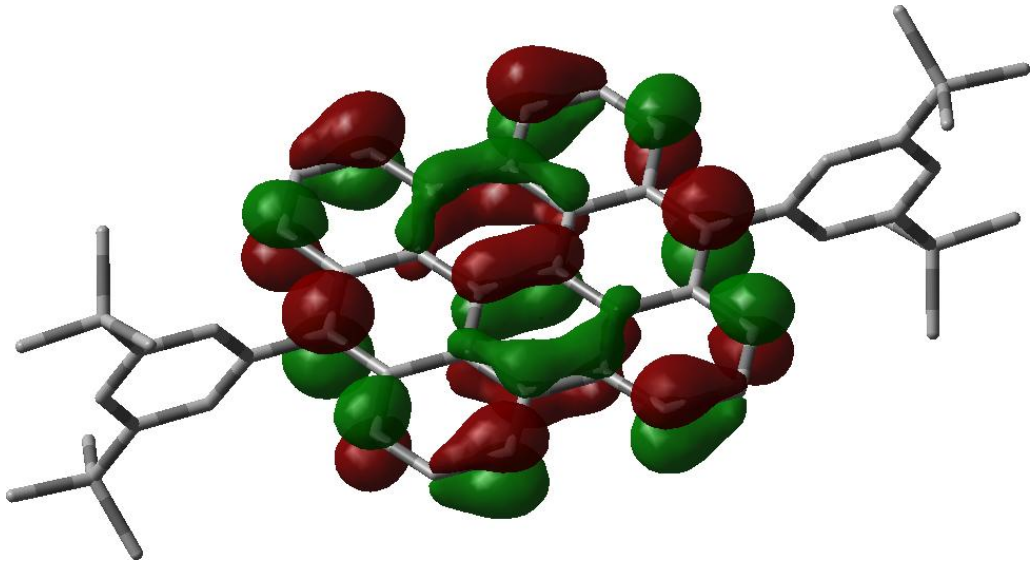
LUMO



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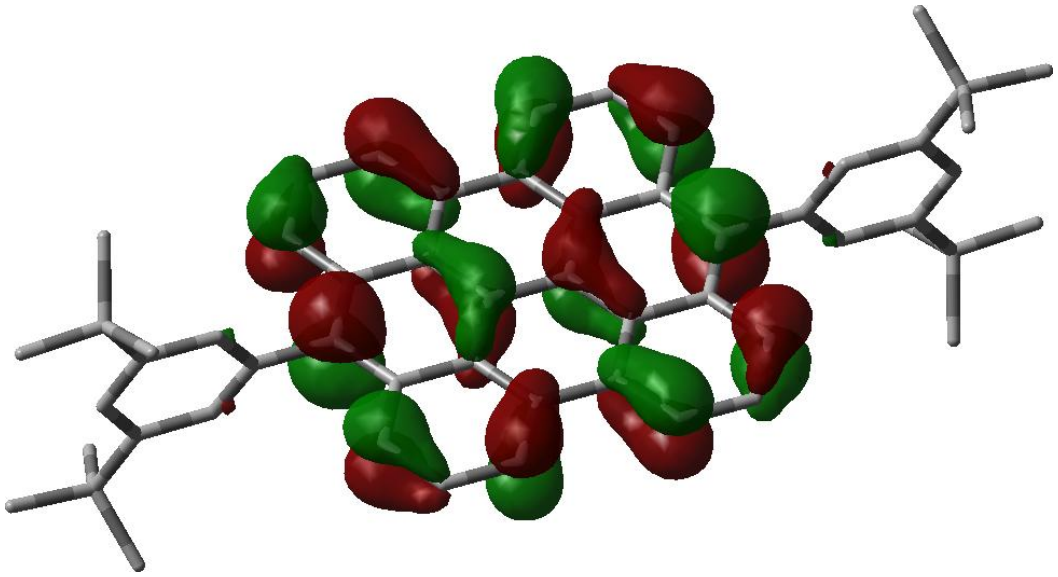

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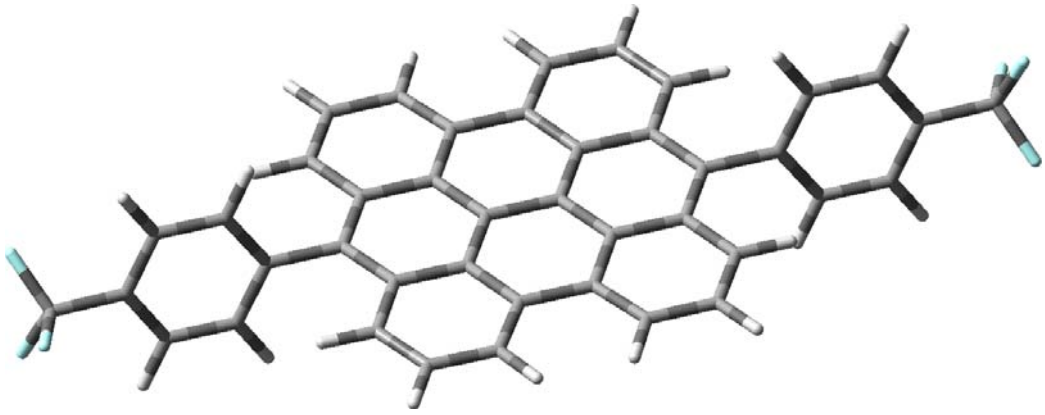

Sum of electronic and zero-point Energies= -2211.212637 (Hartree/Particle)

Sum of electronic and thermal Enthalpies (298.15 K) = -2211.177026

Sum of electronic and thermal Free Energies (298.15 K) = -2211.284760

	X	Y	Z
C	-2.91581199	2.33472772	-3.40745362
C	-2.16568436	1.93186514	-2.30971375
C	-2.12732460	2.77836363	-1.14866355
C	-2.86221322	4.02053015	-1.15488713
C	-3.61963020	4.36675868	-2.31270308
C	-3.63921415	3.54144660	-3.40798454
C	-1.38169141	2.40185390	-0.00306718
C	-2.83393800	4.86218147	-0.02101899
C	-2.09010585	4.49272164	1.12134314
C	-1.35804254	3.24892637	1.13364578
C	-0.60602750	2.88583577	2.30349702
C	-0.60322569	3.74896608	3.39208797
C	-1.30877467	4.96604810	3.37423249
C	-2.03342329	5.33607188	2.27013530

H	-2.96260063	1.71539307	-4.29477253
H	-4.18384291	5.29122562	-2.31621694
H	-4.21871346	3.81374891	-4.28503340
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C	-1.41685965	0.66552647	-2.30090948
C	0.06740039	-0.94124668	-1.11883946
C	0.83627869	-0.47094407	1.15887137
C	0.14016337	1.61795390	2.31350995
C	-1.41641839	-0.19572124	-3.39099306
C	0.01327251	-1.78313300	-2.26882486
C	0.80952747	-1.31168076	0.02430421
C	1.59124532	-0.81864978	2.31784333
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C	-3.08224651	7.28280041	-0.68173163
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C	2.81483002	-2.70300890	-0.60673186
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H	0.09448481	-3.66813687	1.18267625
C	3.52464669	-3.90227742	-0.60305784
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H	4.48943313	-3.96801987	-1.09383819
C	-5.75357754	9.88506557	-0.00422034
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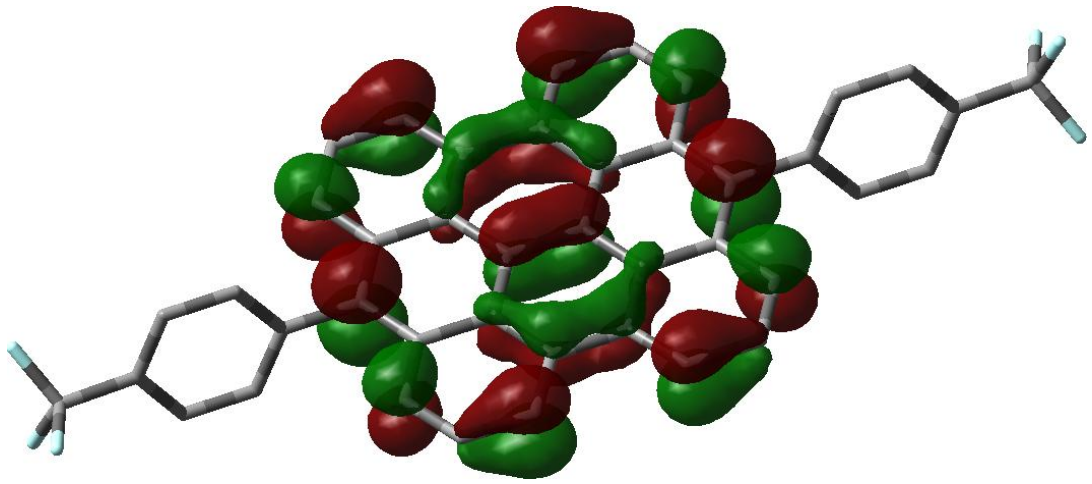
LUMO



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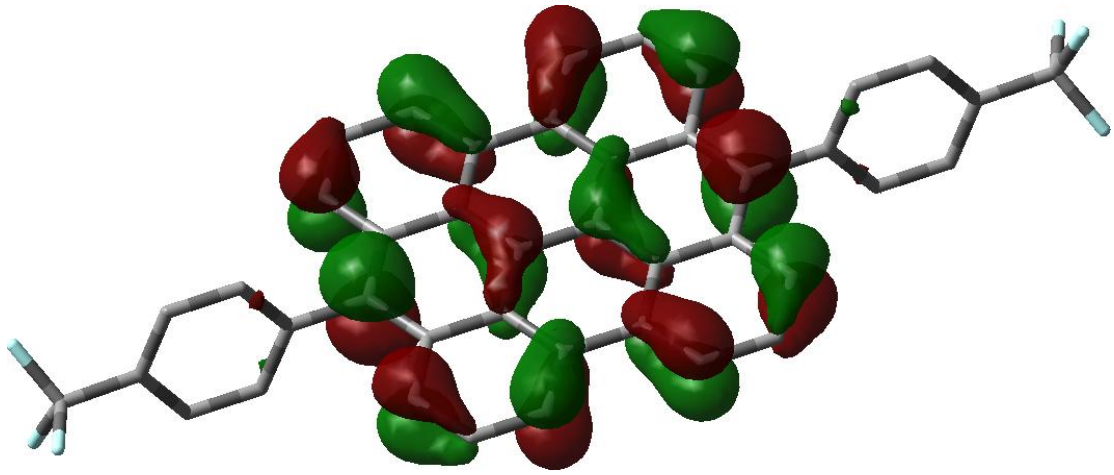

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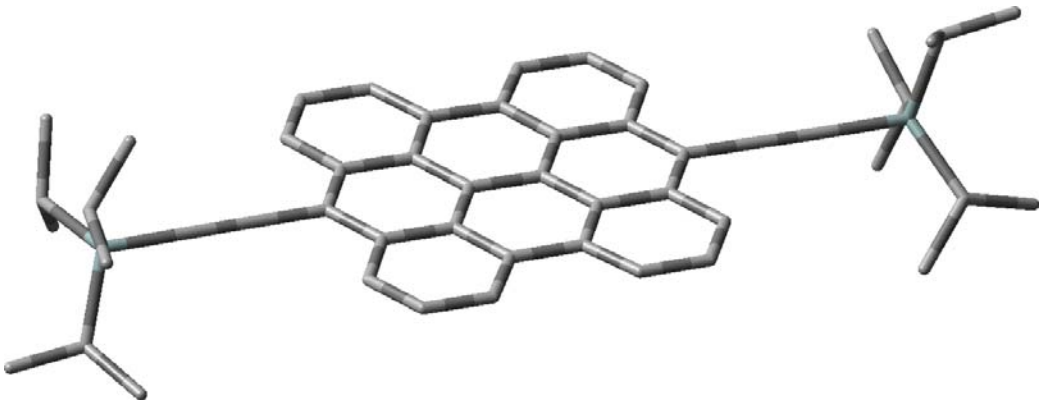

Sum of electronic and zero-point Energies= -2516.095253 (Hartree/Particle)

Sum of electronic and thermal Enthalpies (298.15 K) = -2516.040825

Sum of electronic and thermal Free Energies (298.15 K) = -2516.186476

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C	-1.92502702	2.86928955	-1.18659341
C	-2.64050002	4.11721212	-1.19491560
C	-3.20473982	4.58841822	-2.40980152
C	-3.07172889	3.86193064	-3.56743947
C	-1.34381887	2.38777964	0.01750552
C	-2.77505725	4.86228210	0.00819594
C	-2.19577767	4.38346045	1.21481916
C	-1.47241094	3.13997289	1.21640332
C	-0.88849761	2.67180254	2.44239884
C	-1.05002251	3.43396468	3.59425134
C	-1.75969842	4.64718693	3.58544219
C	-2.32112923	5.11766681	2.42388340
H	-2.29843839	2.09982725	-4.50175457

H	-3.73703201	5.53226794	-2.40266416
H	-3.50276091	4.22867296	-4.49417053
H	-0.62606005	3.10067409	4.53352657
H	-1.86081226	5.21160561	4.50759450
H	-2.86722177	6.05359341	2.40876757
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C	-0.50037353	0.37487302	-1.17392127
C	-0.02918023	0.65599581	1.22425623
C	-1.08656210	0.84166700	-2.39936700
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C	0.69417187	-0.58745500	1.23043872
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C	-0.95483839	0.06252106	-3.54360457
C	0.31250718	-1.62290638	-2.37226605
C	0.80446687	-1.34654787	0.03351520
C	1.29050456	-1.04032759	2.43703670
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C	-0.26139923	-1.15996965	-3.53061903
H	-1.39252541	0.38787956	-4.47935003
H	0.85025777	-2.56354060	-2.35481058
C	1.17611460	-0.30297028	3.58985391
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H	0.40160847	1.45824560	4.52465752
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C	1.50913070	-2.58030245	0.04052198
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H	3.63853121	-5.62619150	2.38797978
C	2.34880772	-6.32437389	-1.36698901
H	2.86465132	-7.29264601	-1.28120833
C	-5.69396688	9.06047268	-1.77266323
H	-6.31388687	9.96701443	-1.68897523
C	-3.88552866	10.14074163	0.57988028
H	-4.30912711	11.05593061	0.13692451
C	-6.60288787	8.46600528	1.12606348
H	-7.18339748	7.71283249	0.57321059
C	5.44796413	-3.79120776	0.72681812
H	6.46787813	-3.49299732	0.45297378
H	4.83865479	-2.88397008	0.78155454
H	5.49985186	-4.21966716	1.73504375
C	5.79764059	-6.03251570	-0.40695461
H	5.43540744	-6.75637562	-1.14518538
H	6.81060264	-5.73739260	-0.70852889
H	5.89063307	-6.55542300	0.55191641
C	3.11423993	-7.59602349	1.72100093
H	4.08365263	-7.83999960	1.27509223
H	3.10220124	-8.02469495	2.73097867
H	2.34559204	-8.11900937	1.14095660
C	1.50581836	-5.78865193	2.47044163
H	1.31221923	-4.71620442	2.55986174
H	0.66222514	-6.22538102	1.92453110

H	1.49611614	-6.21983963	3.47961277
C	2.66852184	-5.74847346	-2.75924801
H	3.74488427	-5.65412402	-2.93441035
H	2.26291865	-6.39328965	-3.54916549
H	2.22490818	-4.75475196	-2.89264334
C	0.83680031	-6.58472275	-1.22497137
H	0.47078189	-7.21430466	-2.04600974
H	0.58934507	-7.09382407	-0.28811258
H	0.26916908	-5.64794757	-1.24981259
C	-6.59782560	7.92639816	-2.29414630
H	-7.47469288	7.76469054	-1.65964087
H	-6.96313073	8.15504909	-3.30327505
H	-6.05365602	6.97675223	-2.35033969
C	-4.57758524	9.36197280	-2.78999288
H	-3.86630815	8.53115933	-2.86427807
H	-4.99915141	9.52071507	-3.79078434
H	-4.01182630	10.26151083	-2.53020669
C	-6.31465920	7.86002520	2.51249428
H	-7.25285062	7.60882238	3.02369775
H	-5.72310312	6.94251732	2.43678869
H	-5.77206942	8.55480017	3.16085507
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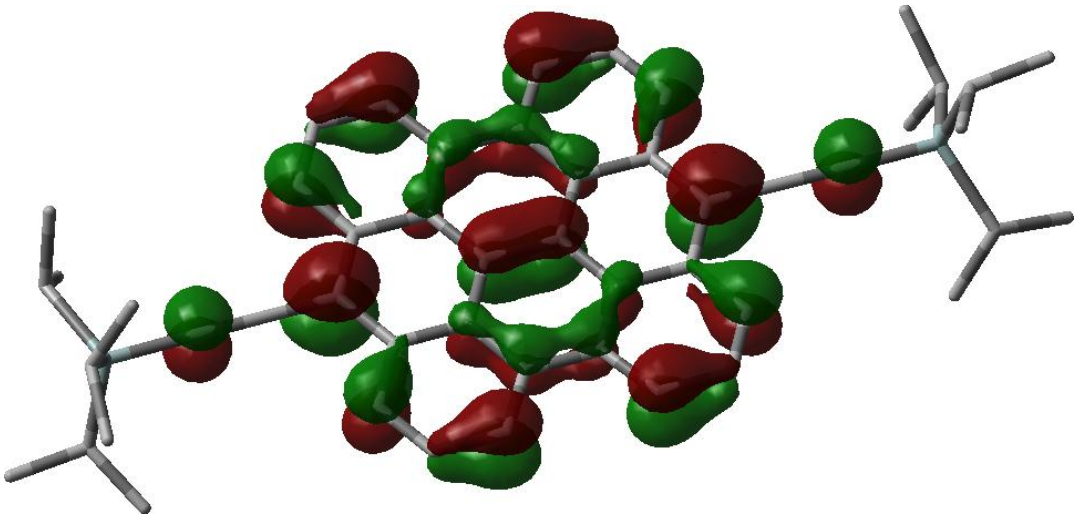
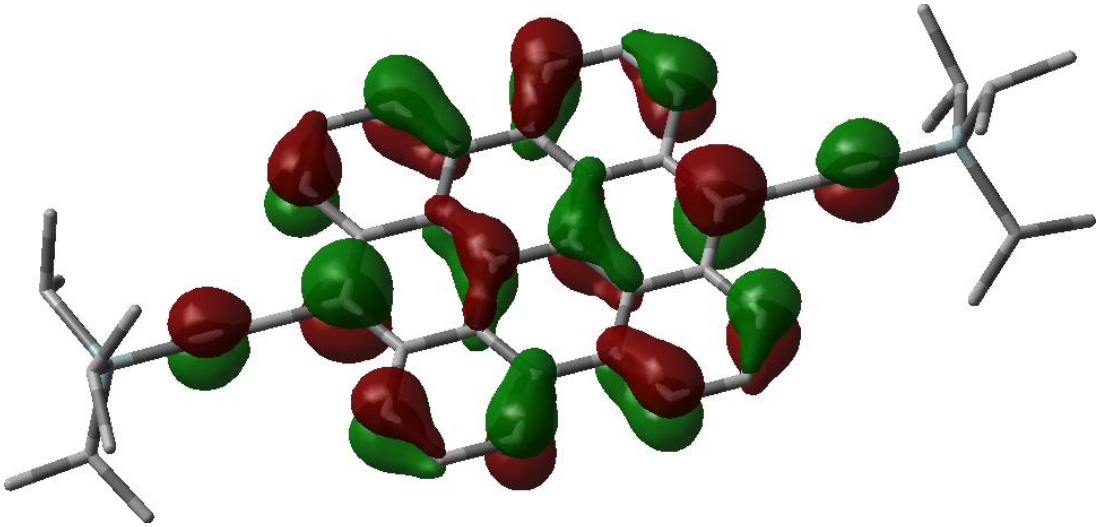
H	-8.40388305	9.50798566	1.79699103
H	-6.97338195	10.53730547	1.76698121
H	-7.78604183	10.11182405	0.25773299
C	-2.45121596	9.97406201	0.03738312
H	-2.41550218	9.88484702	-1.05122911
H	-1.83272071	10.83561279	0.31942138
H	-1.97913404	9.07699931	0.45128381

C	-3.83276563	10.34881550	2.10571674
H	-3.15886528	11.17815711	2.35574289
H	-4.81163534	10.58296072	2.53281230
H	-3.44955513	9.45906248	2.61851311

LUMO



HOMO



6. Appendix: ^{1}H NMR and ^{13}C NMR spectra of all new compounds.

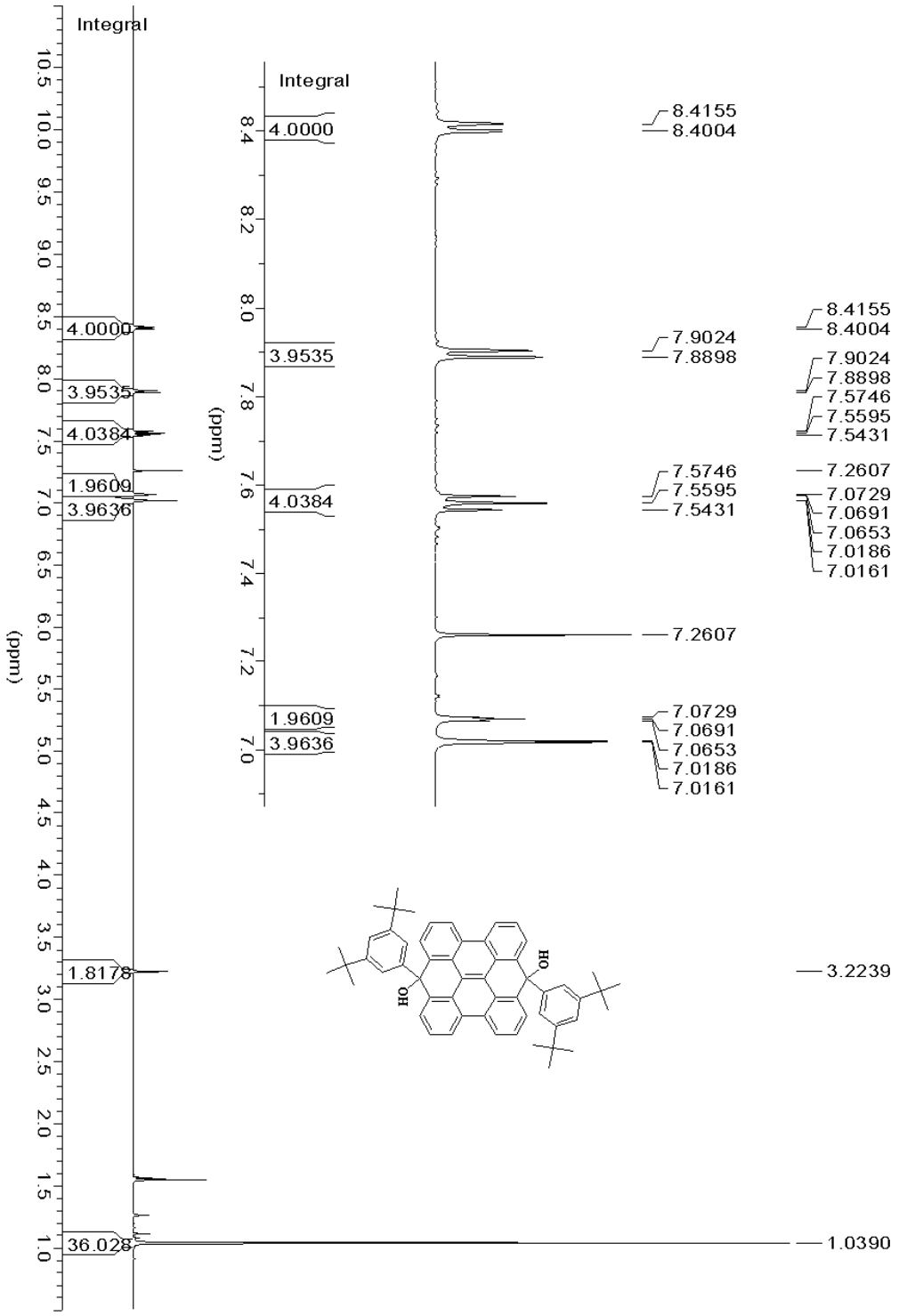


Figure S5. ^{1}H NMR Spectrum ($CDCl_3$) of **8a**

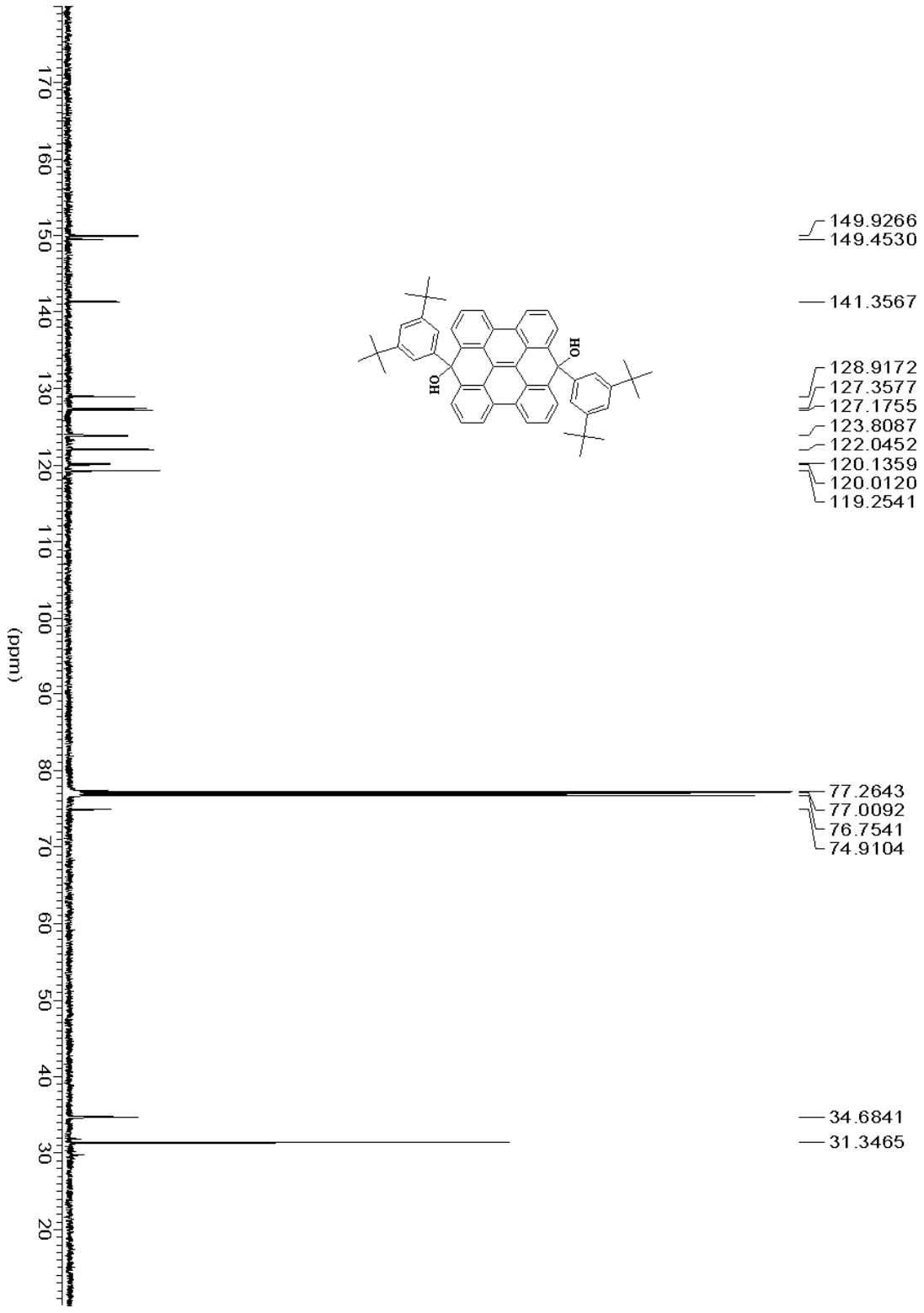


Figure S6. ^{13}C NMR Spectrum ($CDCl_3$) of **8a**

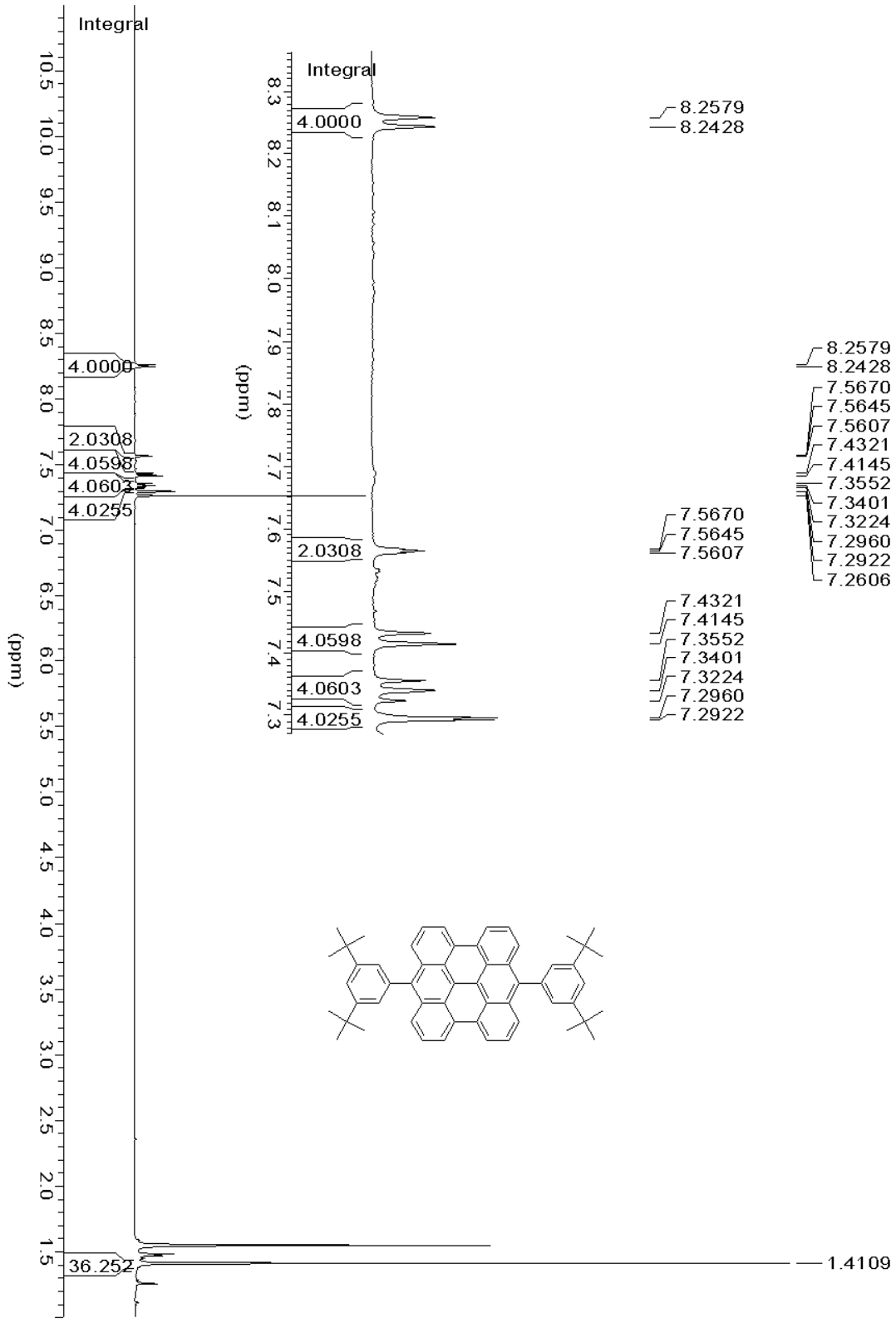


Figure S7. ^{1}H NMR Spectrum ($CDCl_3$) of **4**

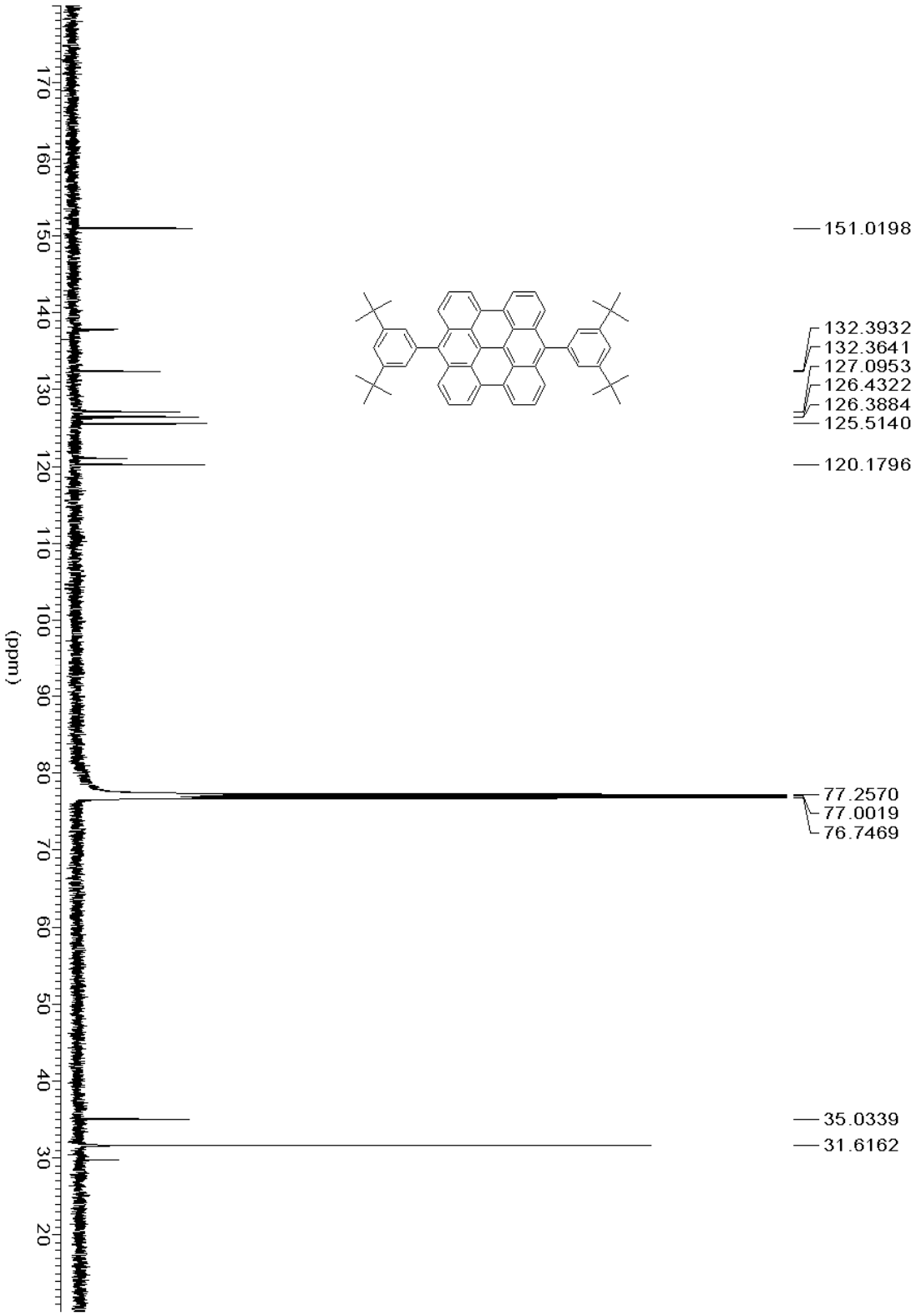


Figure S8. ^{13}C NMR Spectrum ($CDCl_3$) of **4**

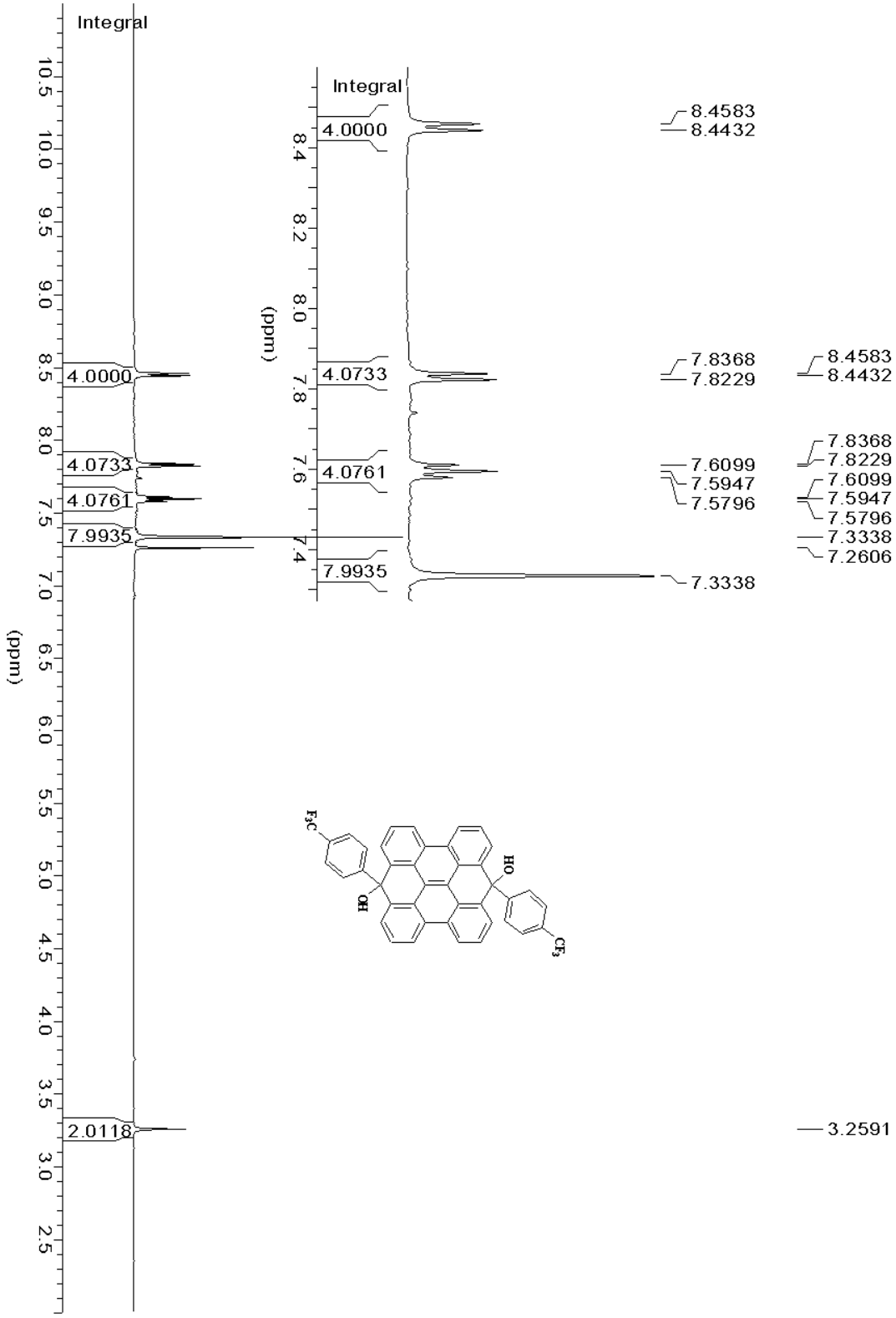


Figure S9. ^{1}H NMR Spectrum ($CDCl_3$) of **8b**

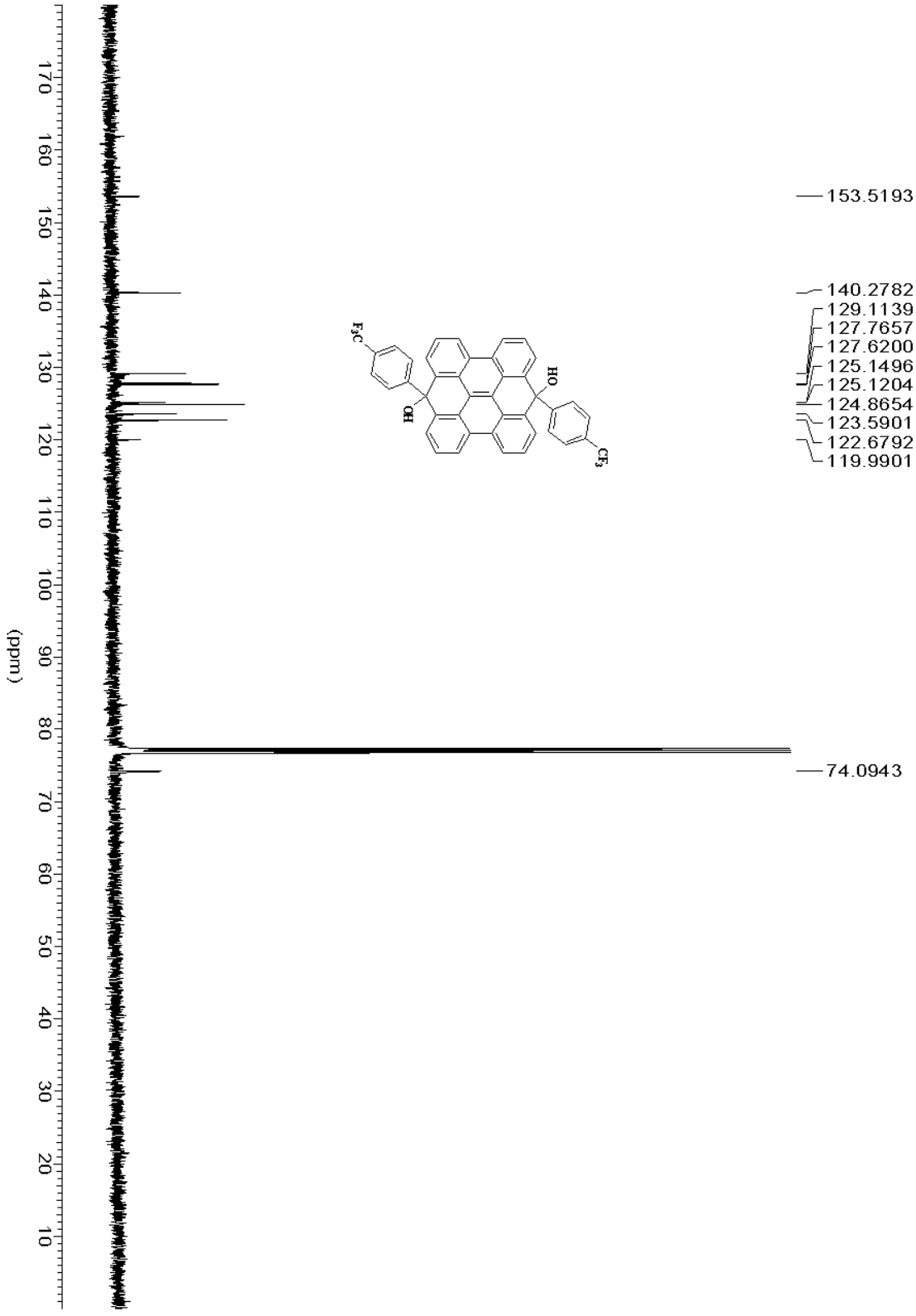


Figure S10. ^{13}C NMR Spectrum ($CDCl_3$) of **8b**

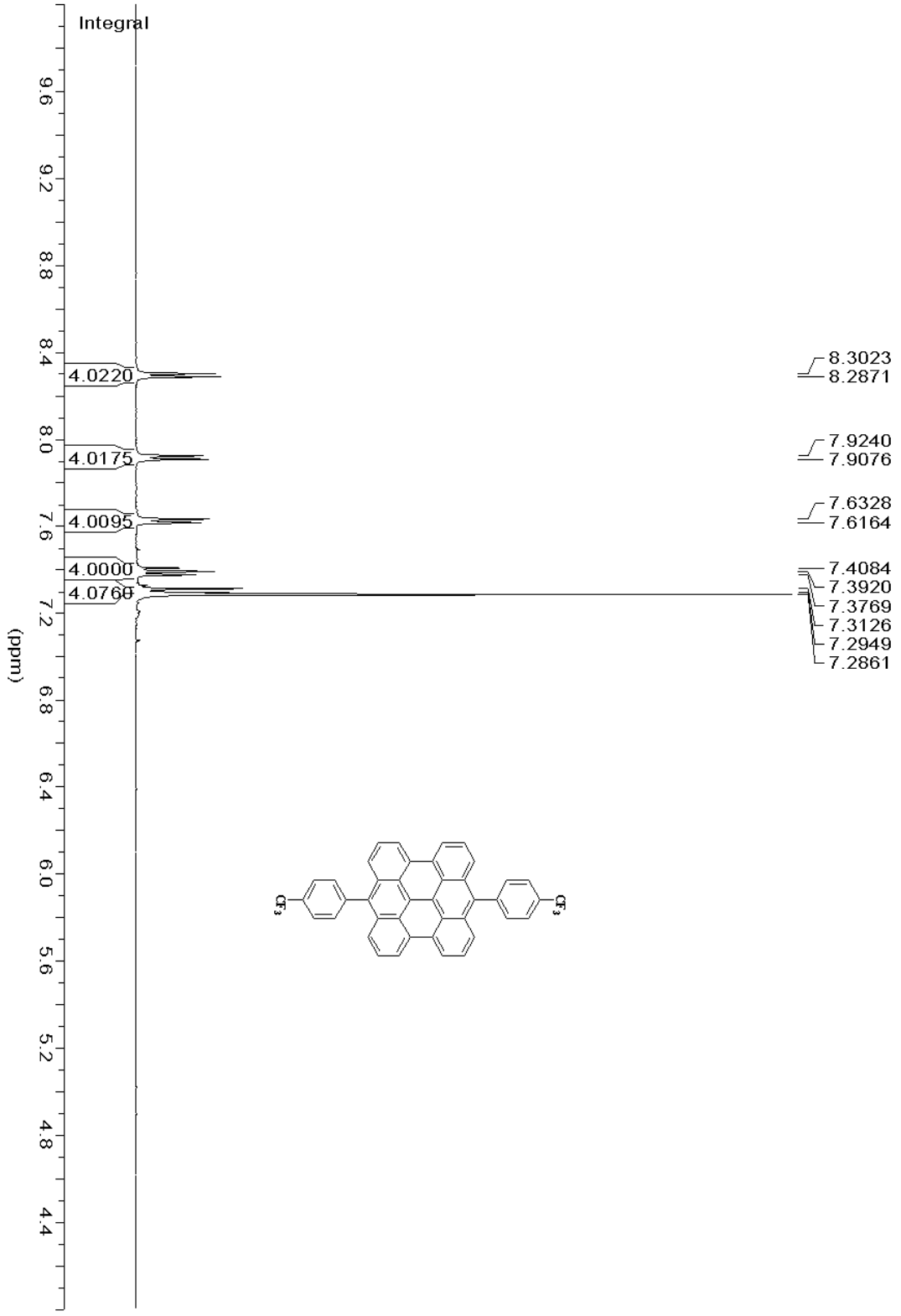


Figure S11. ^{1}H NMR Spectrum ($CDCl_3$) of **5**

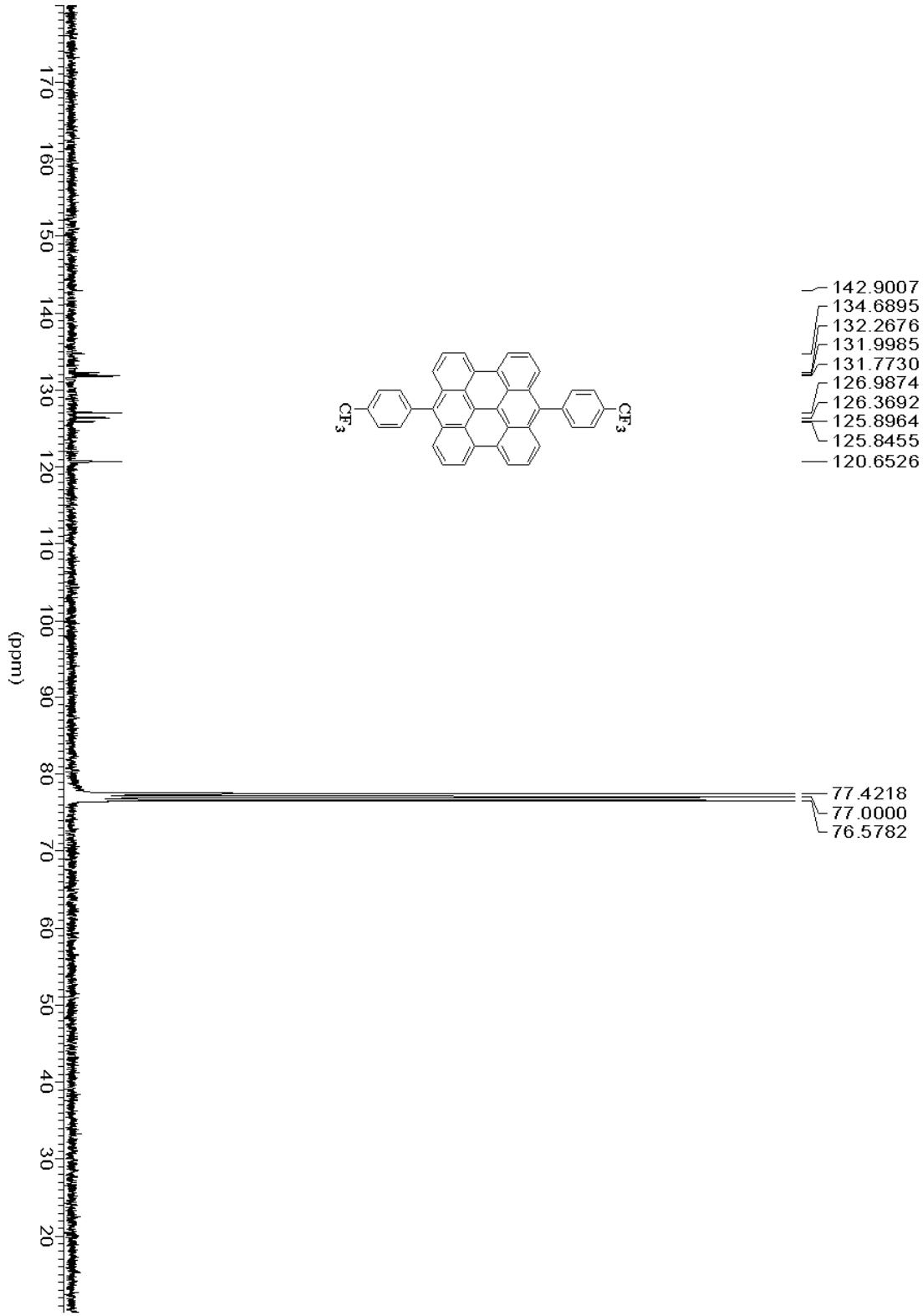


Figure S12. ^{13}C NMR Spectrum ($CDCl_3$) of **5**

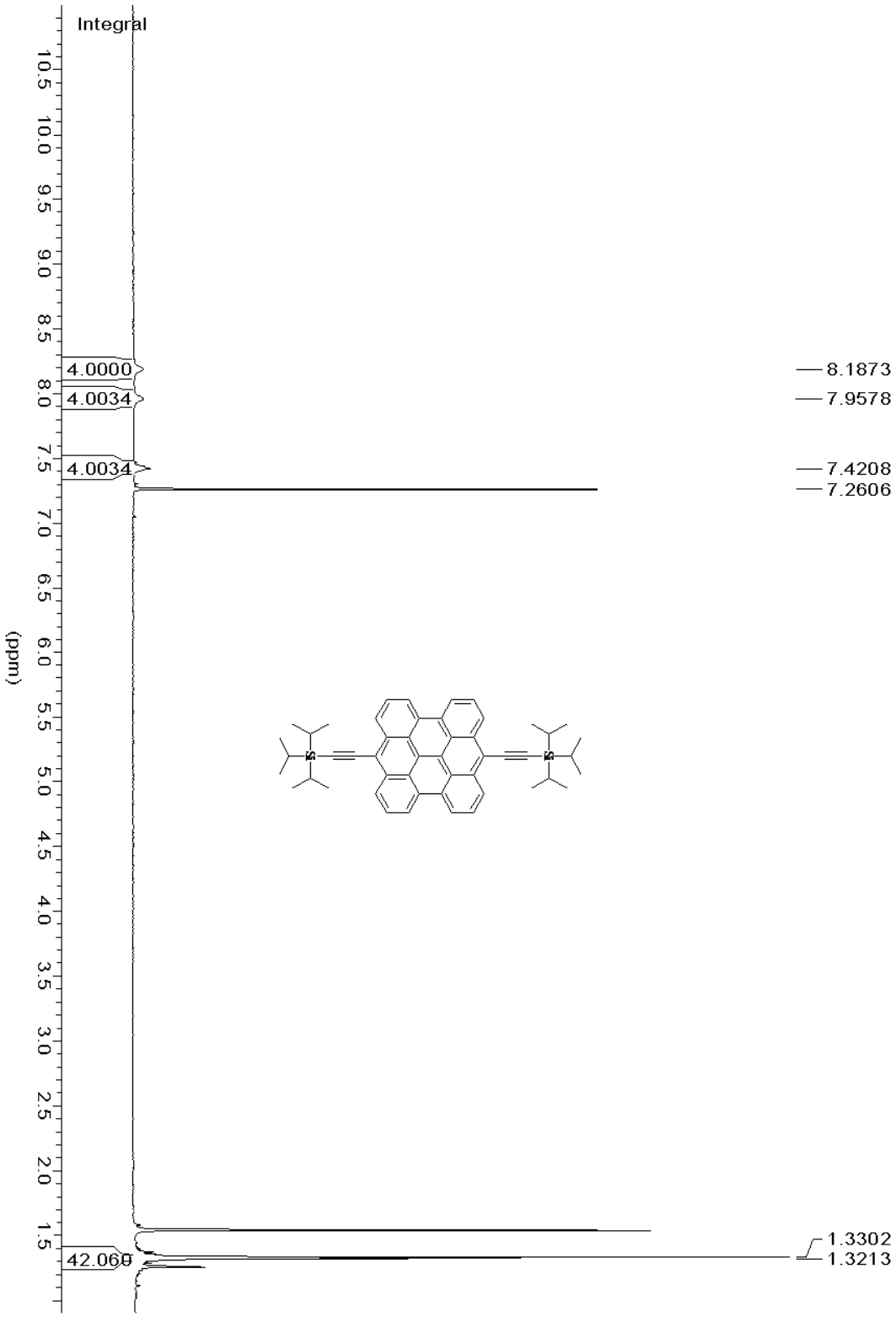


Figure S13. ^{13}C NMR Spectrum ($CDCl_3$) of **6**

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